Benzenamine, N-sulfinyl-

Other names:	Aniline, N-sulfinyl-
	N-Sulfinylaniline
	NSC 40228
	Phenylsulfinylamine
	Phenylthionylamine
	Sulfinylphenylamine
	Sulfurous Imide, phenyl-
	Thionyl imide, phenyl-
	Thionylaniline
	Sulfilimine, phenyl
	N-Thionylaniline
	N-Sulfinylbenzenamine
	N-sulphinylaniline
Inchi:	InChI=1S/C6H5NOS/c8-9-7-6-4-2-1-3-5-6/h1-5H
InchiKey:	FIOJWGRGPONADF-UHFFFAOYSA-N
Formula:	C6H5NOS
SMILES:	O=S=Nc1ccccc1
Mol. weight [g/mol]:	139.18
CAS:	1122-83-4

Physical Properties

Property code	Value	Unit	Source
hf	-56.96	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.715		Crippen Method
mcvol	99.540	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	495.54	K	Joback Method
tc	733.26	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122834&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature